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A CLASS OF OPTIMAL-ORDER ZERO-FINDING METHODS USING DERIVATIVE EVALUATIONS

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A CLASS OF OPTIMAL-ORDER ZERO-FINDING METHODS USING DERIVATIVE EVALUATIONS

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1. INTRODUCTION

It is often necessary to find an approximation to a simple zero ζ of a function f, using evaluations of f and f'. In this paper we consider some methods which are efficient if f' is easier to evaluate than f. Examples of such functions are given in Sections 5 and 6.

The methods considered are stationary, multipoint, iterative methods, "without memory" in the sense of Traub [64]. Thus, it is sufficient to describe how a new approximation (x_1) is obtained from an old approximation (x_0) to ζ. Since we are interested in the order of convergence of different methods, we assume that f is sufficiently smooth near ζ, and that x_0 is sufficiently close to ζ. Our main result is:

<u>Theorem 1.1</u>

There exist methods, of order 2ν, which use one evaluation of f and ν evaluations of f' for each iteration.

By a result of Meersman and Wozniakowski, the order 2ν is the highest possible for a wide class of methods using the same information (i.e., the same number of evaluations of f and f' per iteration): see Meersman [75]. The "obvious"

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interpolatory methods have order $\nu + 1$, but the optimal order 2ν may be obtained by evaluating f' at the correct points. These points are determined by some properties of orthogonal and "almost orthogonal" polynomials.

If $\nu + 1$ evaluations of f are used, instead of one function evaluation and ν derivative evaluations, then the optimal order is 2^ν for methods without memory (Kung and Traub [73,74], Wozniakowski [75a,b]), and $2^{\nu+1}$ for methods with memory (Brent, Winograd and Wolfe [73]). Thus, our methods are only likely to be useful for small ν or if f' is much cheaper than f.

Special Cases

Our methods for $\nu \geq 3$ appear to be new. The cases $\nu = 1$ (Newton's method) and $\nu = 2$ (a fourth-order method of Jarratt [69]) are well known. Our sixth-order method (with $\nu = 3$) improves on a fifth-order method of Jarratt [70].

Generalizations

Generalizations to methods using higher derivatives are possible. One result is:

Theorem 1.2

For $m > 0$, $n \geq 0$, and k satisfying $m + 1 \geq k > 0$, there exist methods which, for each iteration, use one evaluation of $f, f', \ldots, f^{(m)}$, followed by n evaluations of $f^{(k)}$, and have order of convergence $m + 2n + 1$.

The methods described here are special cases of the methods of Theorem 1.2 (take $k = m = 1$, and $\nu = n + 1$) . Since proof of Theorem 1.2 is given in Brent [75], we omit proofs here, and adopt an informal style of presentation. Other possible generalizations are mentioned in Section 7.

2. MOTIVATION

We first consider methods using one evaluation of f, and two of f', per iteration. Let x_0 be a sufficiently good approximation to the simple zero ζ of f, $f_0 = f(x_0)$, and $f_0' = f'(x_0)$. Suppose we evaluate $f'(\tilde{x}_0)$, where

$$\tilde{x}_0 = x_0 - \alpha f_0/f_0' ,$$

and α is a nonzero parameter. Let $Q(x)$ be the quadratic polynomial such that

$$Q(x_0) = f_0 ,$$

$$Q'(x_0) = f_0' ,$$

and

$$Q'(\tilde{x}_0) = f'(\tilde{x}_0) ,$$

and let x_1 be the zero of $Q(x)$ closest to x_0. Jarratt [69] essentially proved:

<u>Theorem 2.1</u>

$$x_1 - \zeta = O(|x_0 - \zeta|^\rho)$$

as $x_0 \to \zeta$, where

$$\rho = \begin{cases} 3 & \text{if } \alpha \neq 2/3 , \\ 4 & \text{if } \alpha = 2/3 . \end{cases}$$

Thus, we choose $\alpha = 2/3$ to obtain a fourth-order method. The proof of Theorem 2.1 uses the following lemma:

<u>Lemma 2.1</u>

If $P(x) = a + bx + cx^2 + dx^3$ satisfies

$$P(0) = P'(0) = P'(2/3) = 0 ,$$

then $P(1) = 0$.

Applying Lemma 2.1, we may show that (for $\alpha = 2/3$)

$$f(x_N) - Q(x_N) = O(\delta^4) ,$$

where

$$x_N = x_0 - f_0/f_0'$$

is the approximation given by Newton's method, and

$$\delta = |f_0/f_0'| = |x_N - x_0| .$$

Now

$$x_N - x_1 = O(\delta^2) ,$$

and

$$f'(x) - Q'(x) = O(\delta^2)$$

for x near x_N , so

$$\begin{aligned} |f(x_1)| &= |f(x_1) - Q(x_1)| \\ &\le |f(x_N) - Q(x_N)| + |f'(\xi) - Q'(\xi)|\cdot|x_N - x_1| \end{aligned}$$

for some ξ between x_N and x_1 . Thus

$$|f(x_1)| = O(\delta^4) + O(\delta^2\cdot\delta^2) = O(\delta^4) ,$$

and

$$x_1 - \zeta = O(|f(x_1)|) = O(\delta^4) = O(|x_0 - \zeta|^4) .$$

3. A SIXTH-ORDER METHOD

To obtain a sixth-order method using one more derivative evaluation than the fourth-order method described above, we need distinct, nonzero parameters, α_1 and α_2 , such that

$$P(0) = P'(0) = P'(\alpha_1) = P'(\alpha_2) = 0$$

implies $P(1) = 0$, for all fifth-degree polynomials

$$P(x) = a + bx + \ldots + fx^5 .$$

Thus, we want the conditions

$$2\alpha_1 c + \ldots + 5\alpha_1^4 f = 0$$

and

$$2\alpha_2 c + \ldots + 5\alpha_2^4 f = 0$$

to imply

$$c + \ldots + f = 0 .$$

Equivalently, we want

$$\mathrm{rank}\begin{bmatrix} 2\alpha_1 & 3\alpha_1^2 & 4\alpha_1^3 & 5\alpha_1^4 \\ 2\alpha_2 & 3\alpha_2^2 & 4\alpha_2^3 & 5\alpha_2^4 \\ 1 & 1 & 1 & 1 \end{bmatrix} = 2 \ ,$$

i.e.,

$$\mathrm{rank}\begin{bmatrix} 1 & \alpha_1 & \alpha_1^2 & \alpha_1^3 \\ 1 & \alpha_2 & \alpha_2^2 & \alpha_2^3 \\ 1/2 & 1/3 & 1/4 & 1/5 \end{bmatrix} = 2 \ ,$$

i.e., for some w_1 and w_2 ,

(3.1) $$w_1\alpha_1^i + w_2\alpha_2^i = 1/(i + 2)$$

for $0 \leq i \leq 3$.

Since $1/(i + 2) = \int_0^1 x^i \cdot x dx$, we see from (3.1) that α_1 and α_2 should be chosen as the zeros of the Jacobi polynomial, $G_2(2, 2, x) = x^2 - 6x/5 + 3/10$, which is orthogonal to lower degree polynomials, with respect to the weight function x , on $[0, 1]$.

Let $y_i = x_0 - \alpha_i f_0/f'_0$, $x_N = x_0 - f_0/f'_0$, $\delta = |f_0/f'_0|$, and let $Q(x)$ be the cubic polynomial such that

$$Q(x_0) = f_0 \ , \quad Q'(x_0) = f'_0 \ ,$$

and

$$Q'(y_i) = f'(y_i)$$

for $i=1,2$. Then

$$f(x) - Q(x) = 0(\delta^4)$$

for x between x_0 and x_N , but

$$f(x_N) - Q(x_N) = 0(\delta^6) \ ,$$

because of our choice of α_1 and α_2 as zeros of $G_2(2, 2, x)$.

(This might be called "superconvergence": see de Boor and Swartz [73].)

A Problem

Since

$$x_N - x_1 = 0(\delta^2)$$

and

$$f'(x) - Q'(x) = 0(\delta^3)$$

for x near x_N, proceeding as above gives

$$|f(x_1)| = 0(\delta^6) + 0(\delta^3 \cdot \delta^2) = 0(\delta^5) ,$$

so the method is only of order five, not six.

A Solution

After evaluating $f'(y_1)$, we can find an approximation $\tilde{x}_N = \zeta + 0(\delta^3)$ which is (in general) a better approximation to ζ than is x_N. From the above discussion, we can get a sixth-order method if we can ensure superconvergence at $\tilde{x}_N$ rather than x_N. Define $\tilde{\alpha}_1$ by

$$\tilde{\alpha}_1(\tilde{x}_N - x_0) = \alpha_1(x_N - x_0) .$$

In evaluating f' at $y_1 = x_0 + \tilde{\alpha}_1(\tilde{x}_N - x_0)$, we effectively used $\tilde{\alpha}_1 = \alpha_1 + 0(\delta)$ instead of α_1, so we must perturb α_2 to compensate for the perturbation in α_1.

From (3.1), we want $\tilde{\alpha}_2$ such that, for some $\tilde{w}_1$ and $\tilde{w}_2$,

(3.2) $$\tilde{w}_1\tilde{\alpha}_1^i + \tilde{w}_2\tilde{\alpha}_2^i = 1/(i + 2)$$

for $0 \leq i \leq 2$. Thus

$$\operatorname{rank}\begin{bmatrix} 1 & \tilde{\alpha}_1 & \tilde{\alpha}_1^2 \\ 1 & \tilde{\alpha}_2 & \tilde{\alpha}_2^2 \\ 1/2 & 1/3 & 1/4 \end{bmatrix} = 2 ,$$

which gives

$$\tilde{\alpha}_2 = (3 - 4\tilde{\alpha}_1)/(4 - 6\tilde{\alpha}_1) = \alpha_2 + O(\delta) .$$

Since

$$\tilde{w}_j = w_j + O(\delta)$$

for $j=1,2$, we have

$$\tilde{w}_1\tilde{\alpha}_1^3 + \tilde{w}_2\tilde{\alpha}_2^3 = 1/5 + O(\delta) . \tag{3.3}$$

(Compare (3.1) with $i = 3$.) If we evaluate f' at $\tilde{y}_2 = x_0 + \tilde{\alpha}_2(\tilde{x}_N - x_0)$, and let x_1 be a sufficiently good approximation to the appropriate zero of the cubic which fits the data obtained from the f and f' evaluations, then (3.2) and (3.3) are sufficient to ensure that the method has order <u>six</u> after all.

4. METHODS OF ORDER 2ν

In this section we describe a class of methods satisfying Theorem 1.1. The special cases $\nu = 2$ and $\nu = 3$ have been given above.

It is convenient to define $n = \nu - 1$. The Jacobi polynomial $G_n(2, 2, x)$ is the monic polynomial, of degree n, which is orthogonal to all polynomials of degree $n - 1$, with respect to the weight function x, on $[0, 1]$. Let $\alpha_1,\ldots,\alpha_n$ denote the zeros of $G_n(2, 2, x)$ in any fixed order. We describe a class of methods of order $2(n + 1)$, using evaluations of $f(x_0)$, $f'(x_0)$, and $f'(y_1),\ldots,f'(y_n)$, where the points $y_1,\ldots,y_n$ are determined during the iteration.

<u>The Methods</u>

1. Evaluate $f_0 = f(x_0)$ and $f'_0 = f'(x_0)$.
2. If $f_0 = 0$ set $x_1 = x_0$ and stop, else set $\delta = |f_0/f'_0|$.
3. For $i=1,\ldots,n$ do steps 4 to 7.

4. Let p_i be the polynomial, of minimal degree, agreeing with the data obtained so far. Let z_i be an approximate zero of p_i, satisfying $z_i = x_0 + O(\delta)$ and $p_i(z_i) = O(\delta^{i+2})$. (Any suitable method, e.g. Newton's method, may be used to find z_i.)

5. Compute $\alpha_{i,j} = \alpha_{i-1,j}\,(z_{i-1} - x_0)/(z_i - x_0)$ for $j=1,\ldots,i-1$. (Skip if $i = 1$.)

6. Let q_i be the monic polynomial, of degree $n + 1 - i$, such that $\int_0^1 P(x)\, q_i(x) \left[\prod_{j=1}^{i-1} (x - \alpha_{i,j})\right] x\,dx = 0$ for all polynomials P of degree $n - i$. (The existence and uniqueness of q_i may be shown constructively: see Brent [75].) Let $\alpha_{i,i}$ be an approximate zero of q_i, satisfying $\alpha_{i,i} = \alpha_i + O(\delta)$ and $q_i(\alpha_{i,i}) = O(\delta^{i+1})$.

7. Evaluate $f'(y_i)$, where

$$y_i = x_0 + \alpha_{i,i}(z_i - x_0) .$$

8. Let p_{n+1} be as at step 4, and x_1 an approximate zero of p_{n+1}, satisfying $x_1 = x_0 + O(\delta)$ and $p_{n+1}(x_1) = O(\delta^{2n+3})$.

Asymptotic Error Constants

The asymptotic error constant of a stationary zero-finding method is defined to be

$$K = \lim_{x_0 \to \zeta} (x_1 - \zeta)/(x_0 - \zeta)^{\rho} ,$$

where ρ is the order of convergence. (Since ρ is an integer for all methods considered here, we allow K to be signed.) Let K_ν be the asymptotic error constant of the methods (of order 2ν) described above. The general form of K_ν is not known, but we have

$$K_1 = \phi_2 ,$$

$$K_2 = \phi_4/9 - \phi_2\phi_3 ,$$

$$K_3 = \phi_6/100 + (1 - 5\alpha_1)\phi_2\phi_5/10 + (3\alpha_1 - 2)\phi_3\phi_4/5 ,$$

and

$$K_4 = \Big\{3\phi_8 - 21\phi_2\phi_7/(1 - \alpha_1) + 9[35(1 - \alpha_3)-3/(1 - \alpha_2)]\phi_3\phi_6 - 25(9 - 44\alpha_3 + 42\alpha_3^2)\phi_4\phi_5\Big\}/3675 ,$$

where

$$\phi_i = \frac{f^{(i)}(\zeta)}{i!f'(\zeta)} .$$

5. RELATED NONLINEAR RUNGE-KUTTA METHODS

The ordinary differential equation

$$dx/dt = g(x) , \quad x(t_0) = x_0 , \tag{5.1}$$

may be solved by quadrature and zero-finding: to find $x(t_0 + h)$ we need to find a zero of

$$f(x) = \int_{x_0}^{x} \frac{du}{g(u)} - h .$$

Note that $f(x_0) = - h$ is known, and $f'(x) = 1/g(x)$ may be evaluated almost as easily as $g(x)$. Thus, the zero-finding methods of Section 4 may be used to estimate $x(t_0 + h)$, then $x(t_0 + 2h)$, etc. When written in terms of g rather than f, the methods are seen to be similar to Runge-Kutta methods.

For example, the fourth-order zero-finding methods of Section 2 (with x_1 an exact zero of the quadratic $Q(x)$) gives:

$$g_0 = g(x_0) ,$$

$$\Delta = hg_0 ,$$

$$g_1 = g(x_0 + 2\Delta/3) ,$$

and

(5.2) $$x_1 = x_0 + 2\Delta/[1 + (3g_0/g_1 - 2)^{\frac{1}{2}}] \ .$$

Note that (5.1) is nonlinear in g_0 and g_1, unlike the usual Runge-Kutta methods. (This makes it difficult to generalize our methods to systems of differential equations.) Since the zero-finding method is fourth-order, $x_1 = x(t_0 + h) + O(h^4)$, so our nonlinear Runge-Kutta method has order three by the usual definition of order (Henrici [62]).

Similarly, any of the zero-finding methods of Section 4 have a corresponding nonlinear Runge-Kutta method. Thus, we have:

Theorem 5.1

If $\nu > 0$, there is an explicit, nonlinear, Runge-Kutta method of order $2\nu - 1$, using ν evaluations of g per iteration, for single differential equations of the form (5.1).

By the result of Meersman and Wozniakowski, mentioned in Section 1, the order $2\nu - 1$ in Theorem 5.1 is the best possible. Butcher [65] has shown that the order of linear Runge-Kutta methods, using ν evaluations of g per iteration, is at most ν, which is less than the order of our methods if $\nu > 1$ (though the linear methods may also be used for systems of differential equations).

6. SOME NUMERICAL RESULTS

In this section we give some numerical results obtained with the nonlinear Runge-Kutta methods of Section 5. Consider the differential equation (5.1) with

(6.1) $$g(x) = (2\pi)^{\frac{1}{2}}\exp(x^2/2)$$

and $x(0) = 0$. Using step sizes $h = 0.1$ and 0.01, we estimated $x(0.4)$, obtaining a computed value x_h. The error e_h was defined by

$$e_h = (2\pi)^{-\frac{1}{2}} \int_0^{x_h} \exp(-u^2/2)du - 0.4 \ .$$

All computations were performed on a Univac 1108 computer, with a floating-point fraction of 60 bits. The results are summarized in Table 6.1. The first three methods are derived from the zero-finding methods of Section 4 (with $\nu = 2, 3$ and 4 respectively). Method RK4 is the classical fourth-order Runge-Kutta method of Kutta [01], and method RK7 is a seventh-order method of Shanks [66].

Table 6.1: Comparison of Runge-Kutta Methods

Method	g evaluations per iteration	Order	$e_{0.1}$	$e_{0.01}$
Sec. 4	2	3	-9.45'-6	1.49'-7
Sec. 4	3	5	3.16'-6	-2.47'-11
Sec. 4	4	7	3.86'-8	3.69'-15
RK4	4	4	1.95'-5	7.90'-9
RK7	9	7	-5.19'-7	-1.67'-13

More extensive numerical results are given in Brent [75]. Note that the differential equation (6.1) was chosen only for illustrative purposes: there are several other ways of computing quantiles of the normal distribution. A practical application of our methods (computing quantiles of the incomplete Gamma and other distributions) is described in Brent [76].

7. OTHER ZERO-FINDING METHODS

In Section 1 we stated some generalizations of our methods (see Theorem 1.2). Further generalizations are described in Meersman [75]. Kacewicz [75] has considered methods which use information about an integral of f instead of a derivative of f .

"Sporadic" methods using derivatives may be derived as in Sections 2 and 3. For example, is there an eighth-order method which uses evaluations of f, f', f'', and f''' at x_0, followed by evaluations of f', f'' and f''' at some point y_1? Proceeding as in Sections 2 and 3, we need a nonzero α satisfying

$$\text{rank}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 4 & 5\alpha & 6\alpha^2 & 7\alpha^3 \\ 12 & 20\alpha & 30\alpha^2 & 42\alpha^3 \\ 24 & 60\alpha & 120\alpha^2 & 210\alpha^3 \end{bmatrix} = 3 ,$$

which reduces to

$$35\alpha^3 - 84\alpha^2 + 70\alpha - 20 = 0 . \tag{7.1}$$

Since (7.1) has one real root, $\alpha = 0.7449...$, an eighth-order method does exist. It is interesting to note that (7.1) is equivalent to the condition

$$\int_0^1 x^3(x - \alpha)^3 dx = 0 .$$

As a final example, we consider sixth-order methods using $f(x_0)$, $f'(x_0)$, $f''(y_1)$, and $f'''(y_2)$. (These could be called Abel-Gončarov methods.) Proceeding as above, we need α_1 and α_2 such that

$$\text{rank}\begin{bmatrix} 2 & 6\alpha_1 & 12\alpha_1^2 & 20\alpha_1^3 \\ 0 & 6 & 24\alpha_2 & 60\alpha_2^2 \\ 1 & 1 & 1 & 1 \end{bmatrix} = 2 ,$$

which gives

$$60\alpha_1^4 - 80\alpha_1^3 + 60\alpha_1^2 - 24\alpha_1 + 3 = 0 \tag{7.2}$$

and

$$\alpha_2 = (1 - 6\alpha_1^2)/(4 - 12\alpha_1) .$$

Fortunately, (7.2) has two real roots, $\alpha_1 = 0.2074...$ and $\alpha_1 = 0.5351...$ Choosing one of these, we may evaluate $f(x_0)$, $f'(x_0)$ and $f''(y_1)$, where y_1 is defined as in Section 3. We may then fit a quadratic to the data, compute the perturbed $\tilde{\alpha}_1$, and take

$$\tilde{\alpha}_2 = (1 - 6\tilde{\alpha}_1^2)/(4 - 12\tilde{\alpha}_1) ,$$

etc., as in Section 3. It is not known whether this method can be generalized, i.e., whether real methods of order $2n$, using evaluations of $f(x_0)$, $f'(x_0)$, $f''(y_1)$, ..., $f^{(n)}(y_{n-1})$, exist for all positive n .

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